Dimethyl succinate 106-65-0 | DTXSID5025152

Model Performance

Model	Data	
Model	Dala	

Weighted KNN model

5-fold CV (75%)		Training (Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.81	0.55	0.81	0.54	0.71	0.61	

Model Results

Predicted value: 27.5 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.14e-01

Confidence level: 5.55e-01

Nearest Neighbors from the Training Set

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1-Methoxy-2-propyl acetate

Measured: 2.29 Predicted: 7.33

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Urea, 1-(p-fluorophenyl)-

Measured: 33.1 Predicted: 49.6

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4-Aminobenzoic acid Measured: 316 Predicted: 96.6

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Urea, (m-fluorophenyl)-

Measured: 58.9 Predicted: 59.1

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(2-Fluorophenyl)urea Measured: 20.9 Predicted: 52.8